



ELSEVIER

Chemical Physics 182 (1994) 409–412

Chemical Physics

Author index to volume 182

- Adamovich, I.V., S.O. Macheret and J.W. Rich, Spatial nonhomogeneity effects in non-equilibrium vibrational kinetics 182 (1994) 167
- Albrecht, U., see H. Schäfer 182 (1994) 53
- Albrecht, U., H. Schäfer and R. Richert, Dispersive first-order reactions. II. Photochromic model system 182 (1994) 61
- Angelié, C., see M. Cauchetier 182 (1994) 375
- Atkinson, G.H., see L. Ujj 182 (1994) 291
- Belford, R.L., see J.M. Canfield 182 (1994) 1
- Bénard, M., see F. Briffaut-Le Guiner 182 (1994) 313
- Billing, G.D. and K.V. Mikkelsen, Dynamical model for S_N2 reactions in solution. The $Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$ reaction 182 (1994) 249
- Bolton, K. and S. Nordholm, Vibrational energy transfer in a one-dimensional chain of diatomic molecules 182 (1994) 263
- Boukheddaden, K., see J. Linares 182 (1994) 225
- Bozek, J.D., see I.H. Suzuki 182 (1994) 81
- Briffaut-Le Guiner, F., P. Plaza, . Nguyen Quy Dao and M. Bénard, Spectroscopic and theoretical studies of 4-nitropyridine N-oxide and of its related charge transfer compounds in their excited state T_1 182 (1994) 313
- Brunger, M.J., see O. Samardzic 182 (1994) 361
- Campargue, A. and D. Permogorov, Intracavity laser absorption spectroscopy of CHD_3 from 10800 to 18000 cm^{-1} 182 (1994) 281
- Canfield, J.M., R.L. Belford, P.G. Debrunner and K.J. Schulten, A perturbation theory treatment of oscillating magnetic fields in the radical pair mechanism 182 (1994) 1
- Cauchetier, M., M. Luce and C. Angelié, Isotopic selectivity in the IR photosensitized dissociation of molecules. I. Generality of the effect 182 (1994) 375
- Charra, F., see D. Markovitsi 182 (1994) 69
- Chattopadhyay, S. and P.L.M. Plummer, Ab initio studies on the mixed heterodimers of ammonia and hydrogen cyanide 182 (1994) 39
- Costa, S.M.B., see P.J.G. Coutinho 182 (1994) 399
- Coutinho, P.J.G. and S.M.B. Costa, The formation of radical ions of ZnTPP in lecithin vesicles evaluated by a global kinetic treatment 182 (1994) 399
- Debrunner, P.G., see J.M. Canfield 182 (1994) 1
- Delaney, J.K., see L. Ujj 182 (1994) 291
- Di Marco, P., see J. Kalinowski 182 (1994) 341

- Doktorov, A.B., see P.A. Purtoy 182 (1994) 149
 Donovan, R.J., see P.J. Wilson 182 (1994) 325
- Ecoffet, C., see D. Markovitsi 182 (1994) 69
- Fattori, V., see J. Kalinowski 182 (1994) 341
 Fiorini, C., see D. Markovitsi 182 (1994) 69
 Fišer, J. and J. Vojtík, Rovibrational dependence of the *ab initio* nuclear quadrupole coupling constants in the $X\ ^3\Sigma^-$ state of NH 182 (1994) 217
- Inokuchi, H., see K. Seki 182 (1994) 353
- Jallabert, C., see D. Markovitsi 182 (1994) 69
- Kalinowski, J., W. Stampor, P. Di Marco and V. Fattori, Electroabsorption study of excited states in hydrogen-bonding solids: epindolidione and linear trans-quinacridone 182 (1994) 341
 Kollmar, C., Localized π electron states in polydiacetylene oligomers 182 (1994) 131
 Kurshid, M.M.P., see M.H. Palmer 182 (1994) 27
- Lawley, K.P., see P.J. Wilson 182 (1994) 325
 Linares, J., K. Boukheddaden and F. Varret, A cooperative two-orbital vibronic model for the solid-state properties of molecular mixed-valence salts and similar ferroelectric solids 182 (1994) 225
 Luce, M., see M. Cauchetier 182 (1994) 375
 Luque, F.J., see M. Orozco 182 (1994) 237
- Macheret, S.O., see I.V. Adamovich 182 (1994) 167
 Markovitsi, D., H. Sigal, C. Ecoffet, P. Millié, F. Charra, C. Fiorini, J.-M. Nunzi, H. Strzelecka, M. Veber and C. Jallabert, Charge transfer in triaryl pyrylium cations. Theoretical and experimental study 182 (1994) 69
 McMahon, M.A. and K.B. Whaley, Variational and diffusion Monte Carlo studies of $(H_2)_N$ clusters 182 (1994) 119
 Mikkelsen, K.V., see G.D. Billing 182 (1994) 249
 Millié, P., see D. Markovitsi 182 (1994) 69
 Molski, A., Generalization of the Smoluchowski theory to include the effect of unimolecular processes: fluorescence quenching 182 (1994) 203
 Mukherjee, P.K., see K. Takeshita 182 (1994) 195
- Nguyen Quy Dao, see F. Briffaut-Le Guiner 182 (1994) 313
 Nordholm, S., see K. Bolton 182 (1994) 263
 Nunzi, J.-M., see D. Markovitsi 182 (1994) 69
- Orozco, M. and F.J. Luque, Optimization of the cavity size for *ab initio* MST-SCRF calculations of monovalent ions 182 (1994) 237
- Palmer, M.H., M.M.P. Kurshid, T.J. Rayner and J.A.S. Smith, Experimental and theoretical studies of the ^{14}N quadrupole tensors in 1H-1, 2, 3-benzotriazole 182 (1994) 27
 Parmentier, J., see H. Vansweevelt 182 (1994) 19

- Permogorov, D., see A. Campargue 182 (1994) 281
- Plaza, P., see F. Briffaut-Le Guiner 182 (1994) 313
- Plummer, P.L.M., see S. Chattopadhyay 182 (1994) 39
- Popov, A.V., see P.A. Purtov 182 (1994) 149
- Popp, A., see L. Ujj 182 (1994) 291
- Purtov, P.A., A.B. Doktorov and A.V. Popov, The Green function method in the theory of nuclear and electron spin polarization. II. The first approximation and its application in the CIDEP theory 182 (1994) 149
- Rayner, T.J., see M.H. Palmer 182 (1994) 27
- Rich, J.W., see I.V. Adamovich 182 (1994) 167
- Richert, R., see H. Schäfer 182 (1994) 53
- Richert, R., see U. Albrecht 182 (1994) 61
- Ridley, T., see P.J. Wilson 182 (1994) 325
- Saito, N., see I.H. Suzuki 182 (1994) 81
- Samardzic, O., E. Weigold, W. von Niessen, V.G. Zakrzewski and M.J. Brunger, Electron momentum spectroscopy of methylamine 182 (1994) 361
- Schäfer, H., U. Albrecht and R. Richert, Dispersive first-order reactions. I. Data analysis 182 (1994) 53
- Schäfer, H., see U. Albrecht 182 (1994) 61
- Schulten, K., see D. Xu 182 (1994) 91
- Schulten, K.J., see J.M. Canfield 182 (1994) 1
- Seki, K., N. Ueno and H. Inokuchi, UV photoemission study of amorphous $n\text{-C}_{36}\text{H}_{74}$ films and their annealing process 182 (1994) 353
- Sigal, H., see D. Markovitsi 182 (1994) 69
- Smith, J.A.S., see M.H. Palmer 182 (1994) 27
- Stampor, W., see J. Kalinowski 182 (1994) 341
- Strzelecka, H., see D. Markovitsi 182 (1994) 69
- Suzuki, I.H., J.D. Bozek and N. Saito, Ionic dissociation of CF_2Cl_2 photoexcited using monochromatic soft X-rays 182 (1994) 81
- Tachikawa, H. and S. Tomoda, A theoretical study on the vibrationally state-selected hydrogen transfer reaction: $\text{NH}^+(v) + \text{NH}_3 \rightarrow \text{NH}_4^+ + \text{NH}_2$. An ab initio MR-SD-CI and classical trajectory approach 182 (1994) 185
- Takeshita, K. and P.K. Mukherjee, Theoretical study on the quasi-bound state and UV spectrum of H_2O_2 with inclusion of the vibrational structure 182 (1994) 195
- Tomoda, S., see H. Tachikawa 182 (1994) 185
- Ueno, N., see K. Seki 182 (1994) 353
- Ujj, L., B.L. Volodin, A. Popp, J.K. Delaney and G.H. Atkinson, Picosecond resonance coherent anti-Stokes Raman spectroscopy of bacteriorhodopsin: spectra and quantitative third-order susceptibility analysis of the light-adapted BR-570 182 (1994) 291
- Van der Vorst, W., see H. Vansweevelt 182 (1994) 19
- Vanquickenborne, L., see H. Vansweevelt 182 (1994) 19
- Vansweevelt, H., L. Vanquickenborne, W. Van der Vorst, J. Parmentier and Th. Zeegers-Huyskens, Theoretical and X-ray photoelectron spectrometric studies of the basicity of a glycine dipeptide 182 (1994) 19

- Varret, F., see J. Linares 182 (1994) 225
Veber, M., see D. Markovitsi 182 (1994) 69
Vojtik, J., see J. Fišer 182 (1994) 217
Volodin, B.L., see L. Ujj 182 (1994) 291
Von Niessen, W., see O. Samardzic 182 (1994) 361
- Weigold, E., see O. Samardzic 182 (1994) 361
Whaley, K.B., see M.A. McMahon 182 (1994) 119
Wilson, P.J., T. Ridley, K.P. Lawley and R.J. Donovan, Double resonance ionisation nozzle cooled spectroscopy (DRINCS) of the $E(^3P_2)$, $f(^3P_0)$ and $f(^1D_2) 0_g^+$ ion-pair states of I_2 182 (1994) 325
- Xu, D. and K. Schulten, Coupling of protein motion to electron transfer in a photosynthetic reaction center: investigating the low temperature behavior in the framework of the spin-boson model 182 (1994) 91
- Zakrzewski, V.G., see O. Samardzic 182 (1994) 361
Zeegers-Huyskens, Th., see H. Vansweevelt 182 (1994) 19



ELSEVIER

Chemical Physics 182 (1994) 413-422

Chemical
Physics

Subject index to volume 182

Methods

Theoretical

Quantized field theory

- Coupling of protein motion to electron transfer in a photosynthetic reaction center: investigating the low temperature behavior in the framework of the spin-boson model, D. Xu and K. Schulten 182 (1994) 91

Many body and quasiparticle approaches

- Variational and diffusion Monte Carlo studies of $(H_2)_N$ clusters, M.A. McMahon and K.B. Whaley 182 (1994) 119

Coupling schemes and perturbative treatments

- A perturbation theory treatment of oscillating magnetic fields in the radical pair mechanism, J.M. Canfield, R.L. Belford, P.G. Debrunner and K.J. Schulten 182 (1994) 1
Localized π electron states in polydiacetylene oligomers, C. Kollmar 182 (1994) 131

Transport quantum mechanics

- The Green function method in the theory of nuclear and electron spin polarization. II. The first approximation and its application in the CIDEP theory, P.A. Purtov, A.B. Doktorov and A.V. Popov 182 (1994) 149

Non-equilibrium thermodynamic and hydrodynamic theories

- Spatial nonhomogeneity effects in nonequilibrium vibrational kinetics, I.V. Adamovich, S.O. Macheret and J.W. Rich 182 (1994) 167
Generalization of the Smoluchowski theory to include the effect of unimolecular processes: fluorescence quenching, A. Molski 182 (1994) 203

Ab initio schemes for stationary properties

- Theoretical and X-ray photoelectron spectrometric studies of the basicity of a glycine dipeptide, H. Vansweevelt, L. Vanquickenborne, W. Van der Vorst, J. Parmentier and Th. Zeegers-Huyskens 182 (1994) 19
Experimental and theoretical studies of the ^{14}N quadrupole tensors in 1H-1, 2, 3-benzotriazole, M.H. Palmer, M.M.P. Kurshid, T.J. Rayner and J.A.S. Smith 182 (1994) 27
Ab initio studies on the mixed heterodimers of ammonia and hydrogen cyanide, S. Chattopadhyay and P.L.M. Plummer 182 (1994) 39

- A theoretical study on the vibrationally state-selected hydrogen transfer reaction: $\text{NH}^+(v) + \text{NH}_3 \rightarrow \text{NH}_4^+ + \text{NH}_2$. An ab initio MR-SD-CI and classical trajectory approach, H. Tachikawa and S. Tomoda 182 (1994) 185
- Theoretical study on the quasi-bound state and UV spectrum of H_2O_2 with inclusion of the vibrational structure, K. Takeshita and P.K. Mukherjee 182 (1994) 195
- Rovibrational dependence of the ab initio nuclear quadrupole coupling constants in the $X^3\Sigma^-$ state of NH, J. Fišer and J. Vojtík 182 (1994) 217
- Computational and simulation methods*
- Dispersive first-order reactions. I. Data analysis, H. Schäfer, U. Albrecht and R. Richert 182 (1994) 53
- Dispersive first-order reactions. II. Photochromic model system, U. Albrecht, H. Schäfer and R. Richert 182 (1994) 61
- Coupling of protein motion to electron transfer in a photosynthetic reaction center: investigating the low temperature behavior in the framework of the spin-boson model, D. Xu and K. Schulten 182 (1994) 91
- Variational and diffusion Monte Carlo studies of $(\text{H}_2)_N$ clusters, M.A. McMahon and K.B. Whaley 182 (1994) 119
- A cooperative two-orbital vibronic model for the solid-state properties of molecular mixed-valence salts and similar ferroelectric solids, J. Linares, K. Boukheddaden and F. Varret 182 (1994) 225
- Optimization of the cavity size for ab initio MST-SCRF calculations of monovalent ions, M. Orozco and F.J. Luque 182 (1994) 237
- Molecular dynamics and scattering theory*
- A theoretical study on the vibrationally state-selected hydrogen transfer reaction: $\text{NH}^+(v) + \text{NH}_3 \rightarrow \text{NH}_4^+ + \text{NH}_2$. An ab initio MR-SD-CI and classical trajectory approach, H. Tachikawa and S. Tomoda 182 (1994) 185
- Dynamical model for $\text{S}_\text{N}2$ reactions in solution. The $\text{Cl}^- + \text{CH}_3\text{Cl} \rightarrow \text{ClCH}_3 + \text{Cl}^-$ reaction, G.D. Billing and K.V. Mikkelsen 182 (1994) 249
- Vibrational energy transfer in a one-dimensional chain of diatomic molecules, K. Bolton and S. Nordholm 182 (1994) 263
- Experimental**
- Infrared spectroscopy*
- Intracavity laser absorption spectroscopy of CHD_3 from 10800 to 18000 cm^{-1} , A. Campargue and D. Permygorov 182 (1994) 281
- Raman spectroscopy*
- Picosecond resonance coherent anti-Stokes Raman spectroscopy of bacteriorhodopsin: spectra and quantitative third-order susceptibility analysis of the light-adapted BR-570, L. Ujj, B.L. Volodin, A. Popp, J.K. Delaney and G.H. Atkinson 182 (1994) 291
- Spectroscopic and theoretical studies of 4-nitropyridine N-oxide and of its related charge transfer compounds in their excited state T_1 , F. Briffaut-Le Guiner, P. Plaza, Nguyen Quy Dao and M. Bénard 182 (1994) 313
- Visible and UV spectroscopy*
- Dispersive first-order reactions. I. Data analysis, H. Schäfer, U. Albrecht and R. Richert 182 (1994) 53

- Dispersive first-order reactions. II. Photochromic model system, U. Albrecht, H. Schäfer and R. Richert 182 (1994) 61
- Theoretical study on the quasi-bound state and UV spectrum of H_2O_2 with inclusion of the vibrational structure, K. Takeshita and P.K. Mukherjee 182 (1994) 195
- Intracavity laser absorption spectroscopy of CHD_3 from 10800 to 18000 cm^{-1} , A. Campargue and D. Permogorov 182 (1994) 281
- Double resonance ionisation nozzle cooled spectroscopy (DRINCS) of the $\text{E}(^3\text{P}_2)$, $\text{f}(^3\text{P}_0)$ and $\text{f}'(^1\text{D}_2)$ 0_g^+ ion-pair states of I_2 , P.J. Wilson, T. Ridley, K.P. Lawley and R.J. Donovan 182 (1994) 325
- Electroabsorption study of excited states in hydrogen-bonding solids: epindolidione and linear trans-quinacridone, J. Kalinowski, W. Stampor, P. Di Marco and V. Fattori 182 (1994) 341
- Fluorescence spectroscopy*
- Charge transfer in triaryl pyrylium cations. Theoretical and experimental study, D. Markovitsi, H. Sigal, C. Ecoffet, P. Millié, F. Charra, C. Fiorini, J.-M. Nunzi, H. Strzelecka, M. Veber and C. Jallabert 182 (1994) 69
- Photoelectron and Auger spectroscopy*
- Theoretical and X-ray photoelectron spectrometric studies of the basicity of a glycine dipeptide, H. Vansweevelt, L. Vanquickenborne, W. Van der Vorst, J. Parmentier and Th. Zeegers-Huyskens 182 (1994) 19
- UV photoemission study of amorphous $n\text{-C}_{36}\text{H}_{74}$ films and their annealing process, K. Seki, N. Ueno and H. Inokuchi 182 (1994) 353
- Electron impact spectroscopy*
- Electron momentum spectroscopy of methylamine, O. Samardzic, E. Weigold, W. von Niessen, V.G. Zakrzewski and M.J. Brunger 182 (1994) 361
- Laser methods*
- Isotopic selectivity in the IR photosensitized dissociation of molecules. I. Generality of the effect, M. Cauchetier, M. Luce and C. Angelié 182 (1994) 375
- The formation of radical ions of ZnTPP in lecithin vesicles evaluated by a global kinetic treatment, P.J.G. Coutinho and S.M.B. Costa 182 (1994) 399
- Picosecond spectroscopy*
- Picosecond resonance coherent anti-Stokes Raman spectroscopy of bacteriorhodopsin: spectra and quantitative third-order susceptibility analysis of the light-adapted BR-570, L. Ujj, B.L. Volodin, A. Popp, J.K. Delaney and G.H. Atkinson 182 (1994) 291
- Non-linear optical spectroscopy*
- Charge transfer in triaryl pyrylium cations. Theoretical and experimental study, D. Markovitsi, H. Sigal, C. Ecoffet, P. Millié, F. Charra, C. Fiorini, J.-M. Nunzi, H. Strzelecka, M. Veber and C. Jallabert 182 (1994) 69
- Synchrotron spectroscopies*
- Ionic dissociation of CF_2Cl_2 photoexcited using monochromatic soft X-rays, I.H. Suzuki, J.D. Bozek and N. Saito 182 (1994) 81

Coherent optical spectroscopy

- Picosecond resonance coherent anti-Stokes Raman spectroscopy of bacteriorhodopsin: spectra and quantitative third-order susceptibility analysis of the light-adapted BR-570, L. Ujj, B.L. Volodin, A. Popp, J.K. Delaney and G.H. Atkinson 182 (1994) 291

Multiple resonance spectroscopy

- Experimental and theoretical studies of the ^{14}N quadrupole tensors in 1H-1, 2, 3-benzotriazole, M.H. Palmer, M.M.P. Kurshid, T.J. Rayner and J.A.S. Smith 182 (1994) 27

Atomic and molecular beam techniques

- Electron momentum spectroscopy of methylamine, O. Samardzic, E. Weigold, W. von Niessen, V.G. Zakrzewski and M.J. Brunger 182 (1994) 361

Time-resolved experiments

- Charge transfer in triaryl pyrylium cations. Theoretical and experimental study, D. Markovitsi, H. Sigal, C. Ecoffet, P. Millié, F. Charra, C. Fiorini, J.-M. Nunzi, H. Strzelecka, M. Veber and C. Jallabert 182 (1994) 69
- Spectroscopic and theoretical studies of 4-nitropyridine N-oxide and of its related charge transfer compounds in their excited state T_1 , F. Briffaut-Le Guiner, P. Plaza, Nguyen Quy Dao and M. Bénard 182 (1994) 313

Mass spectrometry

- Ionic dissociation of CF_2Cl_2 photoexcited using monochromatic soft X-rays, I.H. Suzuki, J.D. Bozek and N. Saito 182 (1994) 81
- Isotopic selectivity in the IR photosensitized dissociation of molecules. I. Generality of the effect, M. Cauchetier, M. Luce and C. Angelié 182 (1994) 375

Mössbauer spectroscopy

- A cooperative two-orbital vibronic model for the solid-state properties of molecular mixed-valence salts and similar ferroelectric solids, J. Linares, K. Boukheddaden and F. Varret 182 (1994) 225

Objects**Bulk systems***Gases*

- Spatial nonhomogeneity effects in nonequilibrium vibrational kinetics, I.V. Adamovich, S.O. Macheret and J.W. Rich 182 (1994) 167
- Theoretical study on the quasi-bound state and UV spectrum of H_2O_2 with inclusion of the vibrational structure, K. Takeshita and P.K. Mukherjee 182 (1994) 195
- Double resonance ionisation nozzle cooled spectroscopy (DRINCS) of the $E(^3\text{P}_2)$, $f(^3\text{P}_0)$ and $f(^1\text{D}_2)$ 0_g^+ ion-pair states of I_2 , P.J. Wilson, T. Ridley, K.P. Lawley and R.J. Donovan 182 (1994) 325

Supersonic beams

- Double resonance ionisation nozzle cooled spectroscopy (DRINCS) of the $E(^3\text{P}_2)$, $f(^3\text{P}_0)$ and $f(^1\text{D}_2)$ 0_g^+ ion-pair states of I_2 , P.J. Wilson, T. Ridley, K.P. Lawley and R.J. Donovan 182 (1994) 325

Liquids mixtures and solutions

- The Green function method in the theory of nuclear and electron spin polarization. II. The first approximation and its application in the CIDEP theory, P.A. Purtov, A.B. Doktorov and A.V. Popov 182 (1994) 149
- Generalization of the Smoluchowski theory to include the effect of unimolecular processes: fluorescence quenching, A. Molski 182 (1994) 203
- Optimization of the cavity size for ab initio MST-SCRF calculations of monovalent ions, M. Orozco and F.J. Luque 182 (1994) 237
- Dynamical model for S_N2 reactions in solution. The $Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$ reaction, G.D. Billing and K.V. Mikkelsen 182 (1994) 249

*Crystals**-neat*

- Experimental and theoretical studies of the ^{14}N quadrupole tensors in 1H-1, 2, 3-benzotriazole, M.H. Palmer, M.M.P. Kurshid, T.J. Rayner and J.A.S. Smith 182 (1994) 27

Glasses

- UV photoemission study of amorphous $n-C_{36}H_{74}$ films and their annealing process, K. Seki, N. Ueno and H. Inokuchi 182 (1994) 353

Polymers

- Dispersive first-order reactions. I. Data analysis, H. Schäfer, U. Albrecht and R. Richert 182 (1994) 53
- Dispersive first-order reactions. II. Photochromic model system, U. Albrecht, H. Schäfer and R. Richert 182 (1994) 61
- Electroabsorption study of excited states in hydrogen-bonding solids: epindolidione and linear trans-quinacridone, J. Kalinowski, W. Stampor, P. Di Marco and V. Fattori 182 (1994) 341

Thin films

- Electroabsorption study of excited states in hydrogen-bonding solids: epindolidione and linear trans-quinacridone, J. Kalinowski, W. Stampor, P. Di Marco and V. Fattori 182 (1994) 341
- UV photoemission study of amorphous $n-C_{36}H_{74}$ films and their annealing process, K. Seki, N. Ueno and H. Inokuchi 182 (1994) 353

Dielectrics

- Electroabsorption study of excited states in hydrogen-bonding solids: epindolidione and linear trans-quinacridone, J. Kalinowski, W. Stampor, P. Di Marco and V. Fattori 182 (1994) 341

Plasmas

- Spatial nonhomogeneity effects in nonequilibrium vibrational kinetics, I.V. Adamovich, S.O. Macheret and J.W. Rich 182 (1994) 167

Biological systems

- A perturbation theory treatment of oscillating magnetic fields in the radical pair mechanism, J.M. Canfield, R.L. Belford, P.G. Debrunner and K.J. Schulten 182 (1994) 1
- Theoretical and X-ray photoelectron spectrometric studies of the basicity of a glycine dipeptide, H. Vansweevelt, L. Vanquickenborne, W. Van der Vorst, J. Parmentier and Th. Zeegers-Huyskens 182 (1994) 19

- Picosecond resonance coherent anti-Stokes Raman spectroscopy of bacteriorhodopsin: spectra and quantitative third-order susceptibility analysis of the light-adapted BR-570, L. Ujj, B.L. Volodin, A. Popp, J.K. Delaney and G.H. Atkinson 182 (1994) 291
- Microscopic systems**
- Molecules (neutral and ionic)*
- Theoretical study on the quasi-bound state and UV spectrum of H_2O_2 with inclusion of the vibrational structure, K. Takeshita and P.K. Mukherjee 182 (1994) 195
- Optimization of the cavity size for ab initio MST-SCRF calculations of monovalent ions, M. Orozco and F.J. Luque 182 (1994) 237
- The formation of radical ions of ZnTPP in lecithin vesicles evaluated by a global kinetic treatment, P.J.G. Coutinho and S.M.B. Costa 182 (1994) 399
- diatomic*
- Rovibrational dependence of the ab initio nuclear quadrupole coupling constants in the $X^3\Sigma^-$ state of NH, J. Fišer and J. Vojtík 182 (1994) 217
- Double resonance ionisation nozzle cooled spectroscopy (DRINCS) of the $E(^3P_2)$, $f(^3P_0)$ and $f(^1D_2)$ 0_g^+ ion-pair states of I_2 , P.J. Wilson, T. Ridley, K.P. Lawley and R.J. Donovan 182 (1994) 325
- small polyatomics*
- Ionic dissociation of CF_2Cl_2 photoexcited using monochromatic soft X-rays, I.H. Suzuki, J.D. Bozek and N. Saito 182 (1994) 81
- A theoretical study on the vibrationally state-selected hydrogen transfer reaction: $\text{NH}^+(\nu) + \text{NH}_3 \rightarrow \text{NH}_4^+ + \text{NH}_2$. An ab initio MR-SD-CI and classical trajectory approach, H. Tachikawa and S. Tomoda 182 (1994) 185
- Dynamical model for $\text{S}_\text{N}2$ reactions in solution. The $\text{Cl}^- + \text{CH}_3\text{Cl} \rightarrow \text{ClCH}_3 + \text{Cl}^-$ reaction, G.D. Billing and K.V. Mikkelsen 182 (1994) 249
- Intracavity laser absorption spectroscopy of CHD_3 from 10800 to 18000 cm^{-1} , A. Campargue and D. Permogorov 182 (1994) 281
- Spectroscopic and theoretical studies of 4-nitropyridine N-oxide and of its related charge transfer compounds in their excited state T_1 , F. Briffaut-Le Guiner, P. Plaza, Nguyen Quy Dao and M. Bénard 182 (1994) 313
- Electron momentum spectroscopy of methylamine, O. Samardzic, E. Weigold, W. von Niessen, V.G. Zakrzewski and M.J. Brunger 182 (1994) 361
- polymeric and biological*
- Coupling of protein motion to electron transfer in a photosynthetic reaction center: investigating the low temperature behavior in the framework of the spin-boson model, D. Xu and K. Schulten 182 (1994) 91
- Localized π electron states in polydiacetylene oligomers, C. Kollmar 182 (1994) 131
- UV photoemission study of amorphous $n\text{-C}_{36}\text{H}_{74}$ films and their annealing process, K. Seki, N. Ueno and H. Inokuchi 182 (1994) 353
- Molecular aggregates*
- Variational and diffusion Monte Carlo studies of $(\text{H}_2)_N$ clusters, M.A. McMahon and K.B. Whaley 182 (1994) 119

-dimers

- Ab initio studies on the mixed heterodimers of ammonia and hydrogen cyanide, S. Chattopadhyay and P.L.M. Plummer 182 (1994) 39
- A theoretical study on the vibrationally state-selected hydrogen transfer reaction: $\text{NH}^+(\nu) + \text{NH}_3 \rightarrow \text{NH}_4^+ + \text{NH}_2$. An ab initio MR-SD-CI and classical trajectory approach, H. Tachikawa and S. Tomoda 182 (1994) 185
- Vibrational energy transfer in a one-dimensional chain of diatomic molecules, K. Bolton and S. Nordholm 182 (1994) 263

-clusters

- Experimental and theoretical studies of the ^{14}N quadrupole tensors in 1H-1, 2, 3-benzotriazole, M.H. Palmer, M.M.P. Kurshid, T.J. Rayner and J.A.S. Smith 182 (1994) 27
- Ab initio studies on the mixed heterodimers of ammonia and hydrogen cyanide, S. Chattopadhyay and P.L.M. Plummer 182 (1994) 39
- Variational and diffusion Monte Carlo studies of $(\text{H}_2)_N$ clusters, M.A. McMahon and K.B. Whaley 182 (1994) 119

-complexes

- Ab initio studies on the mixed heterodimers of ammonia and hydrogen cyanide, S. Chattopadhyay and P.L.M. Plummer 182 (1994) 39

Free radicals (including hydronium and muonium)

- A perturbation theory treatment of oscillating magnetic fields in the radical pair mechanism, J.M. Canfield, R.L. Belford, P.G. Debrunner and K.J. Schulten 182 (1994) 1
- Localized π electron states in polydiacetylene oligomers, C. Kollmar 182 (1994) 131
- The Green function method in the theory of nuclear and electron spin polarization. II. The first approximation and its application in the CIDEP theory, P.A. Purtov, A.B. Doktorov and A.V. Popov 182 (1994) 149
- Rovibrational dependence of the ab initio nuclear quadrupole coupling constants in the $X^3\Sigma^-$ state of NH , J. Fišer and J. Vojtík 182 (1994) 217

Ions and charge carriers

- The formation of radical ions of ZnTPP in lecithin vesicles evaluated by a global kinetic treatment, P.J.G. Coutinho and S.M.B. Costa 182 (1994) 399

Phenomena*Molecular structure*

- Experimental and theoretical studies of the ^{14}N quadrupole tensors in 1H-1, 2, 3-benzotriazole, M.H. Palmer, M.M.P. Kurshid, T.J. Rayner and J.A.S. Smith 182 (1994) 27
- Intracavity laser absorption spectroscopy of CHD_3 from 10800 to 18000 cm^{-1} , A. Campargue and D. Permogorov 182 (1994) 281
- Picosecond resonance coherent anti-Stokes Raman spectroscopy of bacteriorhodopsin: spectra and quantitative third-order susceptibility analysis of the light-adapted BR-570, L. Ujj, B.L. Volodin, A. Popp, J.K. Delaney and G.H. Atkinson 182 (1994) 291

- Spectroscopic and theoretical studies of 4-nitropyridine N-oxide and of its related charge transfer compounds in their excited state T_1 , F. Briffaut-Le Guiner, P. Plaza, Nguyen Quy Dao and M. Bénard 182 (1994) 313
- Vibrations and rotations of molecules*
- Spatial nonhomogeneity effects in nonequilibrium vibrational kinetics, I.V. Adamovich, S.O. Macheret and J.W. Rich 182 (1994) 167
- Theoretical study on the quasi-bound state and UV spectrum of H_2O_2 with inclusion of the vibrational structure, K. Takeshita and P.K. Mukherjee 182 (1994) 195
- Intracavity laser absorption spectroscopy of CHD_3 from 10800 to 18000 cm^{-1} , A. Campargue and D. Permogorov 182 (1994) 281
- Electronic structure and states*
- Ab initio studies on the mixed heterodimers of ammonia and hydrogen cyanide, S. Chattopadhyay and P.L.M. Plummer 182 (1994) 39
- Localized π electron states in polydiacetylene oligomers, C. Kollmar 182 (1994) 131
- Spectroscopic and theoretical studies of 4-nitropyridine N-oxide and of its related charge transfer compounds in their excited state T_1 , F. Briffaut-Le Guiner, P. Plaza, Nguyen Quy Dao and M. Bénard 182 (1994) 313
- Double resonance ionisation nozzle cooled spectroscopy (DRINCS) of the $E(^3P_2)$, $f(^3P_0)$ and $f(^1D_2)$ O_2^+ ion-pair states of I_2 , P.J. Wilson, T. Ridley, K.P. Lawley and R.J. Donovan 182 (1994) 325
- UV photoemission study of amorphous $n-C_{36}H_{74}$ films and their annealing process, K. Seki, N. Ueno and H. Inokuchi 182 (1994) 353
- Electron momentum spectroscopy of methylamine, O. Samardzic, E. Weigold, W. von Niessen, V.G. Zakrzewski and M.J. Brunger 182 (1994) 361
- Electric and magnetic properties*
- A perturbation theory treatment of oscillating magnetic fields in the radical pair mechanism, J.M. Canfield, R.L. Belford, P.G. Debrunner and K.J. Schulten 182 (1994) 1
- Rovibrational dependence of the ab initio nuclear quadrupole coupling constants in the $X^3\Sigma^-$ state of NH, J. Fišer and J. Vojtík 182 (1994) 217
- Electroabsorption study of excited states in hydrogen-bonding solids: epindolidione and linear trans-quinacridone, J. Kalinowski, W. Stampor, P. Di Marco and V. Fattori 182 (1994) 341
- Spin splittings*
- Localized π electron states in polydiacetylene oligomers, C. Kollmar 182 (1994) 131
- The Green function method in the theory of nuclear and electron spin polarization. II. The first approximation and its application in the CIDEP theory, P.A. Purtov, A.B. Doktorov and A.V. Popov 182 (1994) 149
- Molecular interactions*
- Theoretical and X-ray photoelectron spectrometric studies of the basicity of a glycine dipeptide, H. Vansweevelt, L. Vanquickenborne, W. Van der Vorst, J. Parmentier and Th. Zeegers-Huyskens 182 (1994) 19
- Dispersive first-order reactions. I. Data analysis, H. Schäfer, U. Albrecht and R. Richert 182 (1994) 53
- Dispersive first-order reactions. II. Photochromic model system, U. Albrecht, H. Schäfer and R. Richert 182 (1994) 61

- Optimization of the cavity size for ab initio MST-SCRF calculations of monovalent ions,
M. Orozco and F.J. Luque 182 (1994) 237
- Spectral bandshapes and intensities*
- A perturbation theory treatment of oscillating magnetic fields in the radical pair mechanism,
J.M. Canfield, R.L. Belford, P.G. Debrunner and K.J. Schulten 182 (1994) 1
- Coupling of electronic and nuclear motion*
- Coupling of protein motion to electron transfer in a photosynthetic reaction center:
investigating the low temperature behavior in the framework of the spin-boson model,
D. Xu and K. Schulten 182 (1994) 91
- Energy transfer processes*
- Spatial nonhomogeneity effects in nonequilibrium vibrational kinetics, I.V. Adamovich,
S.O. Macheret and J.W. Rich 182 (1994) 167
- Isotopic selectivity in the IR photosensitized dissociation of molecules. I. Generality of the
effect, M. Cauchetier, M. Luce and C. Angelié 182 (1994) 375
- Molecular photophysical processes*
- Charge transfer in triaryl pyrylium cations. Theoretical and experimental study,
D. Markovitsi, H. Sigal, C. Ecoffet, P. Millié, F. Charra, C. Fiorini, J.-M. Nunzi,
H. Strzelecka, M. Veber and C. Jallabert 182 (1994) 69
- Ionic dissociation of CF₂Cl₂ photoexcited using monochromatic soft X-rays, I.H. Suzuki,
J.D. Bozek and N. Saito 182 (1994) 81
- Intramolecular dynamics*
- Vibrational energy transfer in a one-dimensional chain of diatomic molecules, K. Bolton
and S. Nordholm 182 (1994) 263
- vibrational energy redistribution (including vibrational dissociation)*
- Vibrational energy transfer in a one-dimensional chain of diatomic molecules, K. Bolton
and S. Nordholm 182 (1994) 263
- Multiphoton phenomena*
- Isotopic selectivity in the IR photosensitized dissociation of molecules. I. Generality of the
effect, M. Cauchetier, M. Luce and C. Angelié 182 (1994) 375
- Reactions (including dissociation)*
- The Green function method in the theory of nuclear and electron spin polarization. II. The
first approximation and its application in the CIDEP theory, P.A. Purtov, A.B. Doktorov
and A.V. Popov 182 (1994) 149
- gas phase*
- A theoretical study on the vibrationally state-selected hydrogen transfer reaction:
NH⁺ (ν) + NH₃ → NH₄⁺ + NH₂. An ab initio MR-SD-CI and classical trajectory approach,
H. Tachikawa and S. Tomoda 182 (1994) 185
- Isotopic selectivity in the IR photosensitized dissociation of molecules. I. Generality of the
effect, M. Cauchetier, M. Luce and C. Angelié 182 (1994) 375

-condensed phase

- Generalization of the Smoluchowski theory to include the effect of unimolecular processes:
fluorescence quenching, A. Molski 182 (1994) 203
- Dynamical model for S_N2 reactions in solution. The $Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$ reaction,
G.D. Billing and K.V. Mikkelsen 182 (1994) 249

-photochemical

- Dispersive first-order reactions. I. Data analysis, H. Schäfer, U. Albrecht and R. Richert 182 (1994) 53
- Dispersive first-order reactions. II. Photochromic model system, U. Albrecht, H. Schäfer
and R. Richert 182 (1994) 61
- Ionic dissociation of CF_2Cl_2 photoexcited using monochromatic soft X-rays, I.H. Suzuki,
J.D. Bozek and N. Saito 182 (1994) 81
- Generalization of the Smoluchowski theory to include the effect of unimolecular processes:
fluorescence quenching, A. Molski 182 (1994) 203

Electron transfer

- Coupling of protein motion to electron transfer in a photosynthetic reaction center:
investigating the low temperature behavior in the framework of the spin-boson model,
D. Xu and K. Schulten 182 (1994) 91
- The formation of radical ions of ZnTPP in lecithin vesicles evaluated by a global kinetic
treatment, P.J.G. Coutinho and S.M.B. Costa 182 (1994) 399

Ionization (including Rydberg states)

- Electron momentum spectroscopy of methylamine, O. Samardzic, E. Weigold, W. von
Niessen, V.G. Zakrzewski and M.J. Brunger 182 (1994) 361

Structure of solids and liquids

- Variational and diffusion Monte Carlo studies of $(H_2)_N$ clusters, M.A. McMahon and
K.B. Whaley 182 (1994) 119

Phase transitions

- A cooperative two-orbital vibronic model for the solid-state properties of molecular mixed-
valence salts and similar ferroelectric solids, J. Linares, K. Boukheddaden and F. Varret 182 (1994) 225

